

# Universality in Glassy Low-Temperature Physics

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We propose a microscopic translationally invariant glass model which exhibits two level tunneling systems with a broad range of asymmetries and barrier heights in its glassy phase. Their distribution is qualitatively different from what is commonly assumed in phenomenological models, in that symmetric tunneling systems are systematically suppressed. Still, the model exhibits the usual glassy low-temperature anomalies. Universality is due to the collective origin of the glassy potential energy landscape. We obtain a simple explanation also for the mysterious *quantitative* universality expressed in the unusually narrow universal glassy range of values for the internal friction plateau.

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The physics of glassy systems at low temperatures differs strikingly from that of their crystalline counterparts [1]. Differences are observed in thermal properties, in transport phenomena, and in dielectric and acoustic response, and are believed to be due to the existence of tunneling excitations with a broad range of energy splittings and relaxation times, which are absent in crystals. The phenomenological standard tunneling model (STM) [2], and its generalization, the soft potential model (SPM) [3], which paraphrase this idea quantitatively were for many years considered to provide a satisfactory rationalization of glassy low-temperature physics.

Questions into the *origin of the universality* of these phenomena [4] have not yet found clearcut answers; see, however, [5]. In particular, the remarkable degree of *quantitative* universality (e.g., the narrow range of values for sound-attenuation in the 1 K regime) has remained a mystery so far. Also, relations between low- and high-temperature phenomena could not possibly emerge from phenomenological descriptions. Moreover, a number of recent experiments [6, 7, 8] are difficult to reconcile with predictions of prevalent models.

In order to better understand the successes and limitations of the phenomenological approaches, we have recently proposed *microscopic* models for glassy low-temperature physics [9, 10] using heuristics taken from spin-glass theory. The purpose of the present letter is to improve upon [9, 10] with respect to both modeling and scope of analysis. We investigate a glass model described by the Hamiltonian  $H = \sum_i \frac{p_i^2}{2m} + U_{\text{int}}(\{u_i\})$  with a *translationally invariant* interaction energy of the form

$$U_{\text{int}} = \frac{1}{4} \sum_{ij} J_{ij} (u_i - u_j)^2 + \frac{g}{2N} \sum_{ij} (u_i - u_j)^4 \quad (1)$$

The  $u_i$  designate deviations of particle coordinates from some reference positions, and (1) may be thought of as arising from a Born von Karman expansion of the full interaction energy about these positions – taken to be stationary but not necessarily stable. As before [9, 10], glassy properties are modeled by assuming the expan-

sion coefficients at the harmonic level to be Gaussian random couplings with mean  $\overline{J_{ij}} = J_0/N$  and variance  $\overline{(\delta J_{ij})^2} = J^2/N$ . The non-random quartic potential is for stabilization, and so requires  $g > 0$ . Non-translationally invariant versions [9] or models with partial translational invariance [10] have been introduced before.

Our main results are the following. (i) The model exhibits a glassy phase at low temperatures. (ii) The potential energy landscape is represented self-consistently through an ensemble of effective single-site potentials which comprises both single-well potentials (SWPs), and double-well potentials (DWPs), the latter with a broad spectrum of barrier heights and asymmetries. (iii) The distribution of parameters characterizing the single-site potentials depends on the collective state of the system, and differs qualitatively from what is assumed in the phenomenological models. (iv) The model exhibits typical low temperature anomalies, e.g., of the specific heat, and of acoustic or dielectric response. (v) Within the model we can explain, in particular the quantitative universality of glassy low-temperature anomalies expressed e.g. in the unusually narrow range of values for the internal friction plateau. (vi) We also see some unusual frequency dependence of internal friction curves similar to that recently observed in vitreous silica [8].

We now turn to the analysis. Due to the translationally invariant interaction, the system contains global translations as zero modes, and the partition function must be evaluated orthogonal to these modes, i.e. with the constraint  $\sum_i u_i = 0$ . Apart from this detail, the analysis follows standard reasoning. The free energy is obtained by averaging an  $n$ -fold replicated partition sum,  $-\beta f(\beta) = \lim_{N \rightarrow \infty, n \rightarrow 0} (Nn)^{-1} \ln [Z_N^n]_{av}$ , and can be expressed in terms of an Edwards-Anderson matrix of two-replica overlaps  $q_{ab}$ . Although four-replica overlaps must also be introduced during the calculation, the final result does not depend on them. The replica free energy reads

$$n\beta f(\beta) = \frac{(\beta J)^2}{4} \sum_{ab} q_{ab}^2 - 3\beta g \sum_a q_{aa}^2 - \ln \tilde{Z}_n \quad (2)$$

with  $\tilde{Z}_n$  a single-site partition function corresponding to the  $n$ -replica potential  $U_n = \frac{1}{2} \sum_a (J_0 + 12g q_{aa}) u_a^2 - \frac{\beta J^2}{2} \sum_{ab} q_{ab} u_a u_b - \frac{\beta J^2}{8} (\sum_a u_a^2)^2 + g \sum_a u_a^4$ , that is,  $\tilde{Z}_n = \int \prod_a du_a \exp\{-\beta U_n\}$ . The order parameters  $q_{ab}$  must satisfy the fixed point equations  $q_{ab} = \langle u_a u_b \rangle$  with angle brackets denoting a Gibbs average w.r.t. the potential  $U_n$ . As usual, to perform the  $n \rightarrow 0$  limit, one starts from parameterizations of the  $q_{ab}$  matrix based on assumptions concerning transformation properties of solutions under permutation of the replica.

We have looked at the replica symmetric (RS) solution and a solution with one step of replica symmetry breaking (1RSB). Both in RS and 1RSB (and at all higher levels of Parisi's RSB scheme) the system is described by an ensemble of effective single-site potentials of the form

$$U_{\text{eff}}(u) = d_1 u + d_2 u^2 + d_4 u^4, \quad (3)$$

in which  $d_4 = g$  is the coupling constant of the quartic stabilizing interaction, and  $d_1$  and  $d_2$  are randomly varying parameters. We shall occasionally refer to  $d_1$  and  $d_2$  as to an effective local field  $h_{\text{eff}}$  and an effective harmonic coupling  $k_{\text{eff}}$  via  $d_1 = -h_{\text{eff}}$  and  $d_2 = \frac{1}{2}k_{\text{eff}}$ . Their joint distribution is expressed in terms of the order parameters of the system which are in turn obtained in terms of Gibbs averages self-consistently evaluated over the  $U_{\text{eff}}$  ensemble (3). This ensemble of effective single-site potentials is a representation of the glassy potential energy landscape within a mean-field description. Glassy low-temperature anomalies follow from considering the effects of quantized excitations within this ensemble of local potentials.

In RS one assumes  $q_{aa} = q_d$  and  $q_{ab} = q$  for  $a \neq b$ . These must solve the RS fixed point equations

$$q_d = \langle \langle u^2 \rangle \rangle_{\bar{z}, z}, \quad q = \langle \langle u^2 \rangle \rangle_{\bar{z}, z} \quad (4)$$

in which inner brackets denote a Gibbs average w.r.t. the effective single-site potential (3) with

$$\begin{aligned} d_1 &= d_1^{\text{RS}} = -J\sqrt{q}z, \\ d_2 &= d_2^{\text{RS}} = \frac{1}{2}(J_0 + 12g q_d - J^2 C + J \bar{z}), \end{aligned} \quad (5)$$

and  $C = \beta(q_d - q)$ , and outer brackets an average over the zero-mean, unit-variance Gaussians  $\bar{z}$  and  $z$  in  $d_1$  and  $d_2$ . The ensemble of single-site potentials thus comprises both SWPs, and DWPs, the latter with a broad spectrum of barrier heights. A glassy state is signaled by  $q \neq 0$ , thus a non-degenerate distribution of asymmetries of single-site potentials. In the present model the transition is continuous and the critical condition is given by  $1 = (\beta_c J)^2 \langle \langle u^2 \rangle \rangle_{\bar{z}, z}$ , which is just the de Almeida-Thouless condition for the occurrence of a RSB instability. For models with symmetric coupling distributions the transition temperature satisfies  $T_c(J, g) = \frac{J^2}{g} T_c(1, 1)$  with  $k_B T_c(1, 1) \simeq 0.133 E_*$  [11]. In RS,  $d_1$  and  $d_2$  are

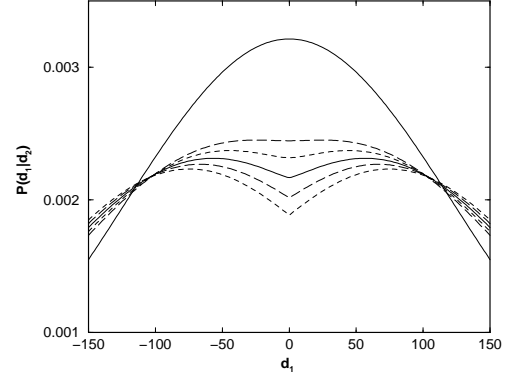


FIG. 1: Central part of  $P(d_1|d_2)$ , for  $J = 50$  and  $g = 1$ . From top to bottom we have RS (independent of  $d_2$ ) and 1RSB with  $d_2 = 10, 5, 0, -5$  and  $-10$ , respectively

Gaussian and uncorrelated. This would be qualitatively in line with assumptions of the SPM, although there are quantitative differences. In contrast to the STM, correlations are predicted between asymmetries and tunneling matrix elements of tunneling systems in DWPs.

The RS solution is unstable and thus strictly not acceptable throughout the glassy phase. For a non-translationally invariant model [9], we have shown RSB effects to be small for the specific heat. Here, we look in greater detail also at the distribution of  $h_{\text{eff}}$  and  $k_{\text{eff}}$ . We shall find it to be *qualitatively* different from what has been obtained in the RS approximation, and thus also from what is assumed in the phenomenological models.

In 1RSB, expected to exhibit the salient RSB effects, one assumes  $q_{aa} = q_d$ ,  $q_{ab} = q_1$  for  $1 < |a - b| \leq m$  and  $q_{ab} = q_0$  for  $|a - b| > m$ . The fixed point equations are now much more complicated, and we shall not reproduce them here. Whereas  $d_2$  has the same form as in RS,  $d_2^{\text{1RSB}} = \frac{1}{2}(J_0 + 12g q_d - J^2 C + J \bar{z})$ , except that now  $C = \beta(q_d - q_1)$ , the local field is more complicated. It is formulated in terms of *two* variables  $z_1$  and  $z_0$

$$d_1 = d_1^{\text{1RSB}} = -J\sqrt{q_1 - q_0} z_1 - J\sqrt{q_0} z_0 \quad (6)$$

of which  $z_0$  is a standard Gaussian, whereas  $z_1$ , while deriving from a Gaussian, becomes correlated with  $z_0$  and  $\bar{z}$  (thus  $d_2$ ) in an intricate way through  $U_{\text{eff}}$ . In the low-temperature limit, to which we restrict our attention here, the result is

$$p(z_1|z_0, \bar{z}) = \frac{\exp\{-z_1^2/2 - D U_{\text{eff}}(\hat{u})\}}{\sqrt{2\pi} \int \mathcal{D}z_1 \exp\{-D U_{\text{eff}}(\hat{u})\}} \quad (7)$$

Here  $D = \beta m$ , which has a finite  $T \rightarrow 0$ -limit,  $\hat{u} = \hat{u}(z_1, z_0, \bar{z})$  is the value of  $u$  which *minimizes*  $U_{\text{eff}}(u)$  for given values of  $z_0$ ,  $z_1$ , and  $\bar{z}$ , and  $\mathcal{D}z_1$  is a Gaussian measure. Fig. 1 displays the resulting distribution of  $d_1$  *conditioned* on  $d_2$ .

The RSB result is *qualitatively* different from the RS result and from what is assumed in phenomenological

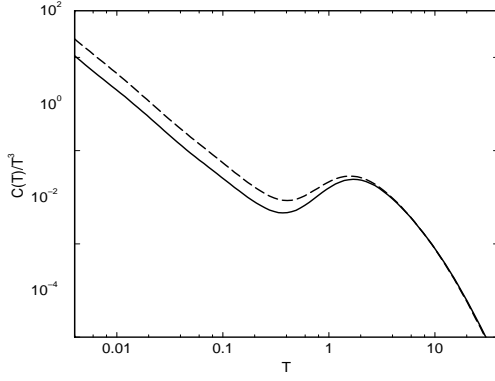


FIG. 2: Low  $T$  specific heat for  $J = 50$  in RS (dashed) and 1RSB (full).

models, in that small  $d_1$  and thus symmetric tunneling systems are systematically suppressed. In fact, in the DWP region for negative  $d_2$  and small  $d_1$ , the form is  $P(d_1, d_2) \simeq \pi_0(d_2)(1 + \pi_1(d_2)|d_1|)$ , so  $P(d_1, d_2)$  is *non-analytic* at  $d_1 = 0$ . Yet, due to the smallness of  $\pi_1(d_2)$ , RSB effects do not have significant influence on functional forms of thermodynamic and response functions at low temperatures. This was observed before for the specific heat in a non-translationally invariant model [9], and is confirmed here.

Glassy low-temperature anomalies follow from low energy excitations in the ensemble of single-site problems  $H_{\text{eff}} = \frac{p^2}{2m} + U_{\text{eff}}(u)$ . The energy of tunneling excitations in DWPs is determined by an asymmetry  $\Delta$  and a tunneling matrix element  $\Delta_0$  as  $E = \sqrt{\Delta^2 + \Delta_0^2}$ , which are in turn expressed through  $d_1$  and  $d_2$  as  $\Delta = E_* d_1 \sqrt{2(|d_2| - 1)}$  and  $\Delta_0 = E_* \sqrt{2}|d_2|^{3/2} \exp\{\frac{2}{3}(1 - |d_2|^{3/2})\}$  [12]. Frequencies of higher (quasi-harmonic) excitations in SWPs or DWPs are given by the curvature of the potential in its minimum,  $U''_{\text{eff}}(u_{\text{min}}) = m\omega^2$  [11].

By averaging over  $P(d_1, d_2)$  one obtains tunneling and vibrational density of states and the specific heat as usual. Tunneling systems give rise to a slightly *super-linear* specific heat at low temperatures,  $C(T) \sim T^{1+\varepsilon}$ , with  $\varepsilon$  decreasing with  $J$  (hence  $T_c$ ),  $\varepsilon \simeq 0.1, 0.05$  and  $0.01$  for  $J = 25, 50$ , and  $100$  respectively, whereas the strongly peaked vibrational density of state is the origin of a Bose-peak in our model; see Fig. 2. RSB effects are small in  $C(T)$ , the dominant effect being a reduction of the tunneling density of states as compared to RS. Except for the super-linearity at low  $T$ , which can be traced down to the translational invariance of the interactions,  $C(T)$  is qualitatively as in [9], both in RS and 1RSB.

It is interesting to compare with assumptions of the STM at the level of the distribution  $P(\Delta, \lambda)$  where  $\lambda = \ln(E_*/\Delta_0)$ . In the STM  $P^{\text{STM}}(\Delta, \lambda) = P_0$  is assumed.

We have

$$P(\Delta, \lambda) = \frac{P(d_1, d_2)}{E_* \sqrt{2(|d_2| - 1)} \left[ \sqrt{|d_2|} - 3/(2|d_2|) \right]} \quad (8)$$

for  $d_2 < -(3/2)^{2/3}$ , with  $d_1 = d_1(\Delta, \lambda)$  and  $d_2 = d_2(\Delta, \lambda)$  instead. Unlike in the STM or the SPM (i) the result is not a constant, and (ii) symmetric tunneling systems are systematically suppressed. If one were to *fit* our results to an STM parameterization one would associate  $P_0 \simeq P(0, \lambda^*)$  for some  $\lambda^* = \mathcal{O}(1) \Leftrightarrow |d_2^*| = \mathcal{O}(10)$ . Interestingly, for reasonable energy scales (associated with tunneling of complexes like  $\text{SiO}_2$  over atomic distances, and giving  $E_*$  between 1 and 5 K), we would estimate  $P_0 = 10^{-7} \dots 10^{-6} \text{ K}^{-1}/\text{Atom}$  for the system with  $J = 50$ , which is the right order of magnitude for typical glasses. Also, using the fact that the low- $T$  limit of the fixed-point equations entails  $q_d, q \propto J$ , and  $C \propto J^{-1}$  in RS, and similarly  $q_d, q_1$  and  $q_0 \propto J$ ,  $C \propto J^{-1}$ , and  $D \propto J^{-2}$  in 1RSB, we can combine this with  $T_c \propto J^2$  and the expression for  $P(d_1, d_2)$  to predict the scaling  $P_0 \sim T_c^{-5/4}$  for large  $T_c$  both in RS and 1RSB, our second result relating low- $T$  properties with a property of the glass-transition in our model. A detailed comparison with experiments is difficult, as a large change in glass transition temperature requires changing composition of the glass, and thus interactions in non-trivial ways. Yet the trend expressed by this result appears to be correct.

Next, we discuss dynamics due to a coupling between local degrees of freedom  $u$  and the strain field  $e$  generated by Debye phonons,  $H_{\text{SB}} = \gamma u e$ , where  $\gamma$  is a deformation potential and  $e = \frac{1}{\sqrt{V}} \sum_{\mathbf{q}, s} \sqrt{\frac{\hbar}{2\rho\omega_{\mathbf{q}, s}}} i q (b_{\mathbf{q}, s} - b_{\mathbf{q}, s}^\dagger)$  the strain-field; the sum is over transversal and longitudinal modes and the tensorial nature of the strain-field is neglected. Quantities like internal friction are obtained by averaging the dynamical susceptibility over the ensemble of single-site problems,

$$Q^{-1} = \frac{\gamma^2}{\rho v^2} \overline{\chi''_{uu}(\omega)}. \quad (9)$$

At low  $T$ , and for  $\hbar\omega \ll k_B T$ , the dominant contribution is the relaxational contribution of tunneling systems in DWPs within the ensemble of single-site potentials. For these a two-level approximation for  $H_{\text{eff}}$  is appropriate and (9) reduces to the well known expression known for two-level tunneling systems, when the internal coordinate  $u$  is approximated by a two state variable in terms of a Pauli matrix,  $u = u_0 \sigma_z$ . Fig. 3 shows the internal friction of the present model for  $J = 50$  and driving frequencies as in [8] computed in 1RSB (except for a different global overall pre-factor, RS results are functionally hardly distinguishable). Unlike in the STM and SPM, the dominant asymptotics is  $Q^{-1} \sim T^{3+\varepsilon}(1 + c_1 T)$  for  $T \ll T^*$  and  $Q^{-1} \simeq \frac{\pi}{2} \frac{P_0 \gamma^2}{\rho v^2} \left( \frac{\hbar\omega}{k_B T} \right)^{\varepsilon/2} (1 + c_2 T)$  for  $T \gg T^*$  — the influence of the  $c_\alpha = \mathcal{O}(10^{-3})$  due to RSB effects being

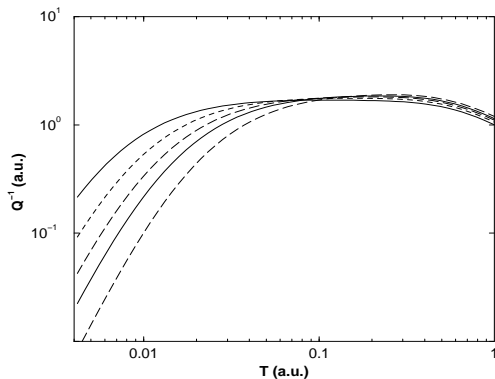


FIG. 3: Internal Friction as a function of  $T$  on a double logarithmic scale for various driving frequencies,  $\omega = 0.33, 1.03, 2.52, 5.03$  and  $14.0$  kHz (top to bottom).

basically indiscernable. The exponent  $\varepsilon$  is that introduced before to quantify the super-linearity of the low- $T$  specific heat, and  $\varepsilon \simeq 0.05$  for the  $J$ -value chosen. Note the following features: (i) there is a slight frequency dependence  $\omega^{\varepsilon/2}$  of the plateau height, correlated with the low- $T$  specific heat exponent (the extra  $T^{-\varepsilon/2}$  factor is indiscernable for the small range of temperatures considered) [13]; (ii) the low  $T$  asymptotics is has by a temperature exponent slightly larger than 3. However, the crossover region from plateau to low-temperature asymptotics is so large that effective exponents in accessible temperature ranges are still *smaller* than 3, the effect being stronger for lower frequencies. Both findings are well in line with recent experiments [8], though observed effective exponents tend to show a somewhat stronger frequency dependence and be smaller than ours.

Lastly, we turn to the universality issue. In [5], universality is explained within a renormalization group approach as a collective effect due to interactions of quantized low-energy excitations. Here it is understood as a property of the interaction-generated glassy potential energy landscape, thus as a collective effect *leading to* a particular spectrum of quantized low-energy excitations. The mechanism is robust and may therefore justly be expected to be insensitive to details. This holds in particular for the tunneling density of states which is driven by a broad distribution of asymmetries and barrier heights. Higher order excitations depend to a larger extent on the shape of the stabilizing potential which is not collectively modified to the same extent, and so a stronger material dependence may be expected in this energy range; this fits well with the observed partial loss of universality in the Bose peak region. Within the present theory there is, beyond a rationalization of universality at the level of exponents, also a rather simple explanation for the mysterious *quantitative* universality of glassy low-temperature physics as expressed in the unusually narrow range of values for the internal friction plateau. It simply follows from combining the scaling  $P_0 \sim J^{-5/2}$  with the plausible

supposition  $\gamma \sim J$  expressing the fact that deformation potential and original interaction are of the same origin, and the elasticity theory scaling  $\rho v^2 \sim J$  for the sound velocity, which together entail  $\frac{P_0 \gamma^2}{\rho v^2} \sim J^{-3/2} \sim T_c^{-3/4}$ . This weak parameter dependence due to cancellations implies, e.g., that the internal friction plateau is changed by only a factor 8 when interaction energies are changed such such as to increase  $T_c$  from 100 to 1600 K!

In summary, we have proposed and analyzed a translationally invariant glass model. It exhibits typical glassy low-temperature anomalies of specific heat and acoustic attenuation. The super-linearity of the low- $T$  specific heat is linked with the non-degenerate barrier-height distribution which in turn can be shown to follow solely from translational invariance (a feature that was absent in our original proposal [9]). Within the model we can correlate low- and high-temperature properties. Universality is understood as consequence of collective effects, and we also have a simple explanation of the mysterious quantitative universality of internal friction data.

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- [1] R.C. Zeller and R.O. Pohl, Phys. Rev. B **4**, 2029 (1971)
  - [2] P.W. Anderson, B.I. Halperin, and C.M. Varma, Philos. Mag. **25**, 1 (1972); W.A. Phillips, J. Low Temp. Phys. **7**, 351 (1972)
  - [3] V.G. Karpov, M.I. Klinger, and F.N. Ignat'ev, Sovj. Phys. JETP **57**, 439 (1983); U. Buchenau, Yu.M. Galperin, V.L. Gurevich, D.A. Parshin, M.A. Ramos, and H.R. Schober, Phys. Rev. B **46**, 2798 (1992)
  - [4] C.C. Yu and A.J. Leggett, Comments Cond. Mat. Phys. **14**, 231 (1988)
  - [5] A.L. Burin and Yu. Kagan, JETP **82**, 159 (1996); Phys. Lett. A **215**, 191 (1996)
  - [6] D. Natelson, D. Rosenberg, and D.D. Osheroff, Phys. Rev. Lett. **80**, 4689 (1998)
  - [7] P. Strehlow, C. Enss, and S. Hunklinger, Phys. Rev. Lett. **80**, 5361 (1998)
  - [8] J. Classen, T. Burkert, C. Enss, and S. Hunklinger, Phys. Rev. Lett. **84**, 2176 (2000)
  - [9] R. Kühn and U. Horstmann, Phys. Rev. Lett. **78**, 4067 (1997)
  - [10] R. Kühn and J. Urmann, J. Phys. C **12**, 6395 (2000)
  - [11] We set the energy scale  $E_*$  by choosing  $g = 1$ , thereby relating  $E_*$  via  $E_* = \hbar^2 / m u_0^2$ , with a mass and length scale  $u_0$  in the problem.
  - [12] M.A. Ramos and U. Buchenau, in: *Tunneling Systems in Amorphous and Crystalline Solids*, P. Esquinazi (Editor), (Springer, Berlin 1998), p. 527
  - [13] The decrease at larger  $T$  is due to the fact that only one phonon processes are considered as in U. Horstmann and R. Kühn, Physica B **263–264**, 290 (1999)